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Coulombic interactions during advection-dominated transport of ions in porous media

Muhammad Muniruzzaman, Lucien Stolze, and Massimo Rolle
Technical University of Denmark (DTU), Environmental Engineering, Kgs. Lyngby, Denmark (masro@env.dtu.dk)

Solute transport of charged species in porous media is significantly affected by the electrochemical migration term resulting from the charge-induced interactions among dissolved ions and with solid surfaces. Therefore, the characterization of such Coulombic interactions and their effect on multicomponent ionic transport is of critical importance for assessing the fate of charged solutes in porous media. In this work we present a detailed investigation of the electrochemical effects during conservative multicomponent ionic transport in homogeneous and heterogeneous domains by means of laboratory bench-scale experiments and numerical simulations. The investigation aims at quantifying the key role of small-scale electrostatic interactions in flow-through systems, especially when advection is the dominant mass-transfer process. Considering dilute solutions of strong electrolytes (e.g., MgCl2 and NaBr) we report results showing the important role of Coulombic interactions in the lateral displacement of the different ionic species for steady-state transport scenarios in which the solutions are continuously injected through different portions of the flow-through chamber [1, 2]. Successively, we focus our attention on transient transport and pulse injection of the electrolytes. In these experiments high-resolution spatial and temporal monitoring of the ions' concentrations (600 samples; 1800 concentration measurements), at closely spaced outlet ports (5 mm), allowed us resolving the effects of charge interactions on the temporal breakthrough and spatial profiles of the cations and anions [3].
The interpretation of the experimental results requires a multicomponent modeling approach with an accurate description of local hydrodynamic dispersion, as well as the explicit quantification of the dispersive fluxes' cross-coupling due to the Coulombic interactions between the charged species. A new 2-D simulator [4], coupling the solution of the multicomponent ionic transport problem with the geochemical code PHREEQC has been developed and used to quantitatively interpret the experimental results.

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